On the Representations of Overtones of Degenerate Vibrational Fundamentals. (I)

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— Abstracts of Papers —

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37. On the Representations of Overtones of Degenerate Vibrational Fundamentals. (I).

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In order to determine the representations of the nuclear-vibrational term in the polyatomic systems with spatial symmetries Tisza[1] obtained the recursion formulas between characters of representations of successive overtones. As the bases of these representations were, however, the n-th products of the Hermite polynomial, the solution of the n-dimensional isotropic oscillator by the orthogonal displacement coordinates, then it was not possible to verify the correspondence of the irreducible representation with the quantum number of the nuclear angular momentum. Therefore it is necessary to solve the Schroedinger equation for the system mentioned above by the polar coordinates of n-dimensional displacement space. The transformation properties of the overtones of the triply degenerate fundamental are determined by the spherical harmonics (as the bases), which are especially equivalent to the problem treated in the crystal systems[2] So we have given the irreducible representations of all other degenerate vibrational levels[3], and further the detailed consideration to the fact that the symmetry group of the system is isomorphic to the unimodular unitary group in n dimension with (n^2-1) parameters, where the total nuclear angular momentum is defined as follows:

$$L^2 = \sum_{\mu \neq \nu}^{\kappa} L_{\mu\nu}^2 \left[\kappa = \binom{n}{2}\right], \quad L_{\mu\nu} = \frac{\hbar}{i}\left(x_\mu \frac{\partial}{\partial x_\nu} - x_\nu \frac{\partial}{\partial x_\mu}\right)$$

Under the transformations of this group the eigenspaces of the Hamiltonian transform according to the representations by symmetric tensor, and then we can obtain these irreducible ingredients.

1) L. Tisza, Zeits. f. Phys. 82, 48 (1933).

2) H. A. Bethe, Ann. d. Phys. 3, 133 (1929); F. C. Von der Lage and H. A. Bethe, Phys. Rev. 71, 612 (1947).

3) There is a special treatment in "Quantum Theory of Molecules" in Japanese (1950).